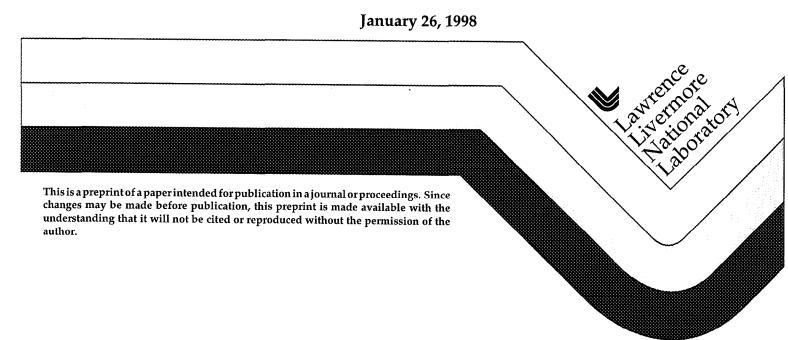
## The Dielectric Boundary Condition for the Embedded Curved Boundary (ECB) Method

D. W. Hewett C. S. Kueny

This paper was prepared for and presented at the
16th International Conference on Numerical Simulation of Plasmas
Santa Barbara, California
February 9-12, 1998



#### DISCLAIMER

This document was prepared as an account of work sponsored by an agency of the United States Government Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

# The Dielectric Boundary Condition for the

### Embedded Curved Boundary (ECB) Method

Dennis W. Hewett and Christopher S. Kueny D&NT, LLNL, Livermore CA 94551

A new version of ECB1 has been completed that allows nonuniform grid spacing and a new dielectric boundary condition. ECB was developed to retain the simplicity and speed of an orthogonal mesh while capturing much of the fidelity of adaptive, unstructured finite element meshes. Codes based on orthogonal meshes are easy to work with and lead to well-posed elliptic and parabolic problems that are comparatively easy to solve. Generally, othogonal mesh representations lead to banded matrices while unstructured representations lead to more complicated sparse matrices. Recent advances in adapting banded linear systems to massively parallel computers reinforce our opinion that iterative field solutions utilizing banded matrix methods will continue to be competitive<sup>2</sup>. Unfortunately, the underlying "stair-step" boundary representation in simple orthogonal mesh (and recent Adaptive Mesh Refinement) applications is inadequate. With ECB, the curved boundary is represented by piece-wise-linear representations of curved internal boundaries embedded into the orthogonal mesh-we build better, but not more, coefficients in the vicinity of these boundaries-and we use the surplus free energy on more ambitious physics models.

ECB structures are constructed out of the superposition of analytically prescribed building blocks. In 2-D, we presently use a POLY4 (linear boundaries defined by 4 end points), an ANNULUS, (center, inner & outer radii, starting & stopping angle), a ROUND (starting point & angle, stopping point & angle, fillet radius). A link-list AIRFOIL has also been constructed. In the ECB scheme, we first find each intercept of the structure boundary with an I or J grid line is assigned an index K. We store the actual x,y value at the intercept, and the slope of the boundary at that intercept, in arrays whose index K is associated with the corresponding mesh point just inside the structure. In 2-D, a point just outside a structure may have up to 4 intercepts associated with it. We now construct PieceWise Linear Segments (PWLS)-from the slope and intercept—that will serve as the computational boundary—a boundary constructed as a superposition of the analytic elements given as input.

The intersection of these PWLSs with other nearby PWLSs define the endpoints. We insist that there be an endpoint within each cell for each sequence
of PWLSs coming through that cell. We give directionality to a PWLS by the
convention that looking from point 1 to point 2 will place the interior of the
structure on the left. This scheme allows the generalization to those boundary structures that do not actually have any mesh points inside a structure<sup>1</sup>.
Since these structures are defined by their analytically defined bounding walls,
points can always be found that are "inside" a given wall segment—even though
it may, in fact, be outside the opposite bounding segment. Such subgrid geometry is useful, for example, in a gun configuration with a thin electrode, perhaps

not parallel to any axes of the orthogonal mesh, in which the electrode simply contributes to an external focusing field.

#### ECB Coefficients for Elliptic Equations

For simplicity, we consider a 1D Poisson equation. The equation is

$$\frac{\partial \epsilon \partial S}{\partial x^2} = \frac{\epsilon_p \frac{S_{i+1} - S}{\Delta_p} - \epsilon_m \frac{S - S_{i-1}}{\Delta_m}}{(\Delta_m + \Delta_p)/2} = -\rho$$

where  $\Delta_m = x_i - x_{i-1}$ ,  $\Delta_p = x_{i+1} - x_i$ , and  $\epsilon_m = (\epsilon_i + \epsilon_{i-1})/2$ ,  $\epsilon_p = (\epsilon_{i+1} + \epsilon_i)/2$ . Defining  $\Delta \equiv (\Delta_m + \Delta_p)/2$ ,

$$\epsilon_n S_n / \Delta_n \Delta - S \left[ \epsilon_n / \Delta_n + \epsilon_m / \Delta_m \right] / \Delta + \epsilon_m S_m / \Delta_m \Delta = -\rho , \qquad (1)$$

we first form and store coefficients for all points I as if there were no boundaries, then redefine "smarter" coefficients that describe the boundary constraints at those points just outside of a structure.

#### **Dirichlet Boundary Conditions**

Consider a location i just outside of (below) a structure intercept

$$S_m$$
  $S_m$   $S_p$   $S_i$   $S_p$ 

For Dirichlet boundary conditions, we specify the value B at that intercept  $S_i$  by using (1) as if it had a closer mesh point for the i+1 location

$$S_i = B, \quad \epsilon(B - S)/\delta_p \Delta - \epsilon_m (S - S_m)/\Delta_m \Delta = -\rho$$

The coefficients for a tridiagonal matrix at points i and i+1 (and all other interior points) are

$$i \qquad i+1, interior$$

$$S_{p}: \qquad 0 \qquad 0$$

$$S \qquad (\epsilon_{m}/\Delta_{m}\Delta + \epsilon/\delta_{p}\Delta) \qquad 1$$

$$S_{m}: \qquad \epsilon_{m}/\Delta_{m}\Delta \qquad 0$$

$$rhs: \qquad -\rho - \epsilon B/\delta_{p}\Delta \qquad B$$

$$(2)$$

#### **Dielectric Boundary Conditions**

Consider again the location i just outside of (below) a structure intercept. We wish to impose the first-order dielectric condition

$$\left| \epsilon \frac{\partial S}{\partial x} \right|_{1}^{2} = \epsilon_{p1} \frac{S_{p} - S_{i}}{\Delta_{p} - \delta_{p}} - \epsilon \frac{S_{i} - S}{\delta_{p}} = \sigma \tag{3}$$

where  $\epsilon_{p1}$ ,  $\epsilon$  are evaluated at points i+1 and i. We now solve for  $S_i$  and use it with (1), again as if it had a shorter leg in the templet. Solving for  $S_i$  and plugging into (1) gives

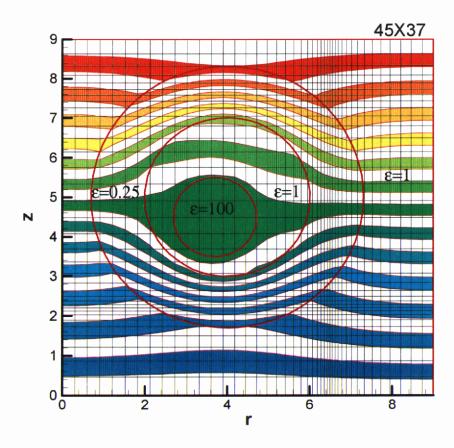
$$\left[\frac{\epsilon_{i+1}\delta_p S_p + (\epsilon S - \sigma \delta_p) (\Delta_p - \delta_p)}{\Delta_{ED}} - \epsilon S\right] / \delta_p \Delta - \epsilon_m (S - S_m) / \Delta_m \Delta = -\rho$$

where  $\epsilon \Delta_{ED} \equiv [\epsilon_{i+1} \delta_p + \epsilon (\Delta_p - \delta_p)]$  The equations simplifies leading to coefficients

$$i \qquad i+1 \\ S_{p}: \qquad \epsilon_{i+1}/\Delta_{ED}\Delta \qquad \qquad \epsilon'_{p}/\Delta'_{p}\Delta' \\ S \qquad -\left[\epsilon_{i+1}/\Delta_{ED} + \epsilon_{m}/\Delta_{m}\right]/\Delta \qquad -\left[\epsilon'_{p}/\Delta'_{p} + \epsilon'_{i-1}/\Delta'_{ED}\right]/\Delta' \qquad (4) \\ S_{m}: \qquad \epsilon_{m}/\Delta_{m}\Delta \qquad \qquad \epsilon'_{i-1}/\Delta'_{ED}\Delta' \\ rhs: \qquad -\rho + \frac{\sigma(\Delta_{p} - \delta_{p})}{\Delta_{ED}\Delta} \qquad -\rho' + \frac{\sigma'(\Delta'_{m} - \delta'_{m})}{\Delta'_{ED}\Delta'}$$

where  $\epsilon' \Delta_{ED}' \equiv \left[ \epsilon_{i-1}' \delta_m' + \epsilon' \left( \Delta_m' - \delta_m' \right) \right]$  and the other 'coefficients have analogous definitions when viewed from the i+1 point. The full, unmodified coefficients are solved in the interior of the dielectric. The generalization to 2D is quite straightforward, leading to the introduction of a simple cosine of the intercept of the PWLS into the effective surface charge. The construction of the gradients is more tedious but also straightforward and is described in Ref 1

An example of this dielectric condition is shown the contour plot below. S lines tend to be compressed in regions with  $\epsilon < 1$  and excluded from regions where  $\epsilon$  is large Dielectric boundary conditions on the ECB interfaces. On the left and right are Neumann zero boundary conditions while Dirichlet boundary conditions are used on the top (S=constant) and bottom (S=0). Notice that the solution is better than the contour plotter; the solution is computed on the mesh points using the precise location of the boundary intercept; the contour plotter interpolates only between mesh points



Additionally, since ECB does not change the matrix structure but only the element values near a structure, any linear system solver may be used without modification.

#### References

- 1) D.W. Hewett, "The Embedded Curved Boundary Method for Orthogonal Meshes", J. Comp. Phys. (in press, 1998).
- 2) M.A. Lambert, G.L. Rodrigue, and D.W. Hewett, "A Parallel DSDADI Method for Solution of the Steady State Diffusion Equation", (accepted Parallel Computing), 1997.

Work performed under the auspices of the U.S. D.O.E. by LLNL under Contract W-7405-Eng-48.